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Point-defect Structure of GaN:Er

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Beamline(s): X15B

The absorption minimum of silica-based fibers in the 1.54-μm Er-luminescence region, coupled with the low thermal quenching behavior of wide-band-gap hosts, makes GaN:Er an important system for potential optoelectronics applications. X-ray absorption measurements show that Er replaces Ga in GaN as a point defect in concentrations as high as $\gtrsim 10^{21}$ Er/cm^3, i.e., $\gtrsim$1 at. %. A Er–N bond length of 2.17 ± 0.02 Å was determined, which is shorter than that in bulk ErN by 0.25 Å. This is the shortest measured bond length between Er in a compound and any other atom, including H. The reason for such a short bond is traceable to the relatively ionic Er–N bonds and unusually low coordination number in GaN:Er. The size and bonding of Er in GaN is similar to that of Er^{3+} ion in ErN, and summing the ionic radii for 6-fold coordinated Er^{3+} (0.89 Å) and N^{3-} (1.46 Å) only slightly underestimates the Er–N distance in ErN (with a rocksalt structure). The same sum, however, is considerably larger than the Er–N distance in GaN:Er. Correcting these radii for their anomalously low 4-fold coordination in GaN (see Fig. 1), however, viz., 0.78 and 1.44 Å, brings their sum into much closer agreement with experiment. This picture is supported by first-principles calculations, which yield a Er–N bond length of 2.20 Å (the 1.5% larger value than experiment is consistent with the 1.6% overestimate of the GaN lattice parameters obtained with these theoretical methods). The relatively low energy penalty calculated for substituting Er for Ga is also consistent with the picture of small lattice distortion as depicted in Fig. 2.

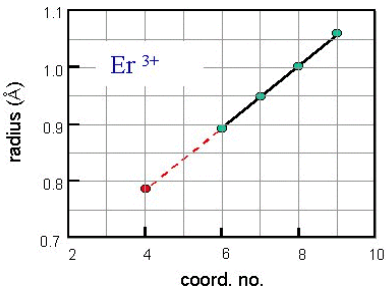

Figure 1. Extrapolation of ionic radius versus coordination number. A similar extrapolation is applicable to N^{3-}.

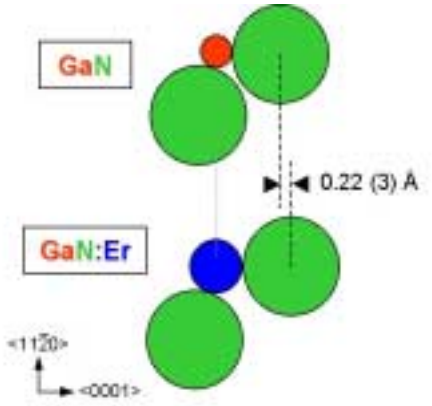

Figure 2. View in the (110) plane of nearest neighbor distances, showing the small distortion around Er by substitutional occupation of a Ga site in GaN.